4-Cyclohexylphenylacetic acid 35889-00-0 | DTXSID60189446

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.09

Global applicability domain: Inside

Local applicability domain index: 3.17e-01

Confidence level: 8.17e-01

Nearest Neighbors from the Training Set

Image not found

1-Naphthaleneacetic acid

Measured: 2.95 Predicted: 3.47

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4-tert-Butylbenzoic acid

Measured: 4.57 Predicted: 3.53

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3-Hydroxy-2-naphthoic acid

Measured: 3.98 Predicted: 3.94

Image not found

Benzilic acid
Measured: 1.82
Predicted: 3.42

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Benzoic acid, 4-(methylamino)-

Measured: 2.40 Predicted: 4.00